

SUPPLEMENTARY MATERIAL

We model the amphiphiles as discrete Gaussian chains having a solvophilic block and two solvophobic tails. For each block, the harmonic potential for the chain connectivity takes the form

$$h_i(\{\mathbf{r}\}) = \frac{3kT}{2b^2} \sum_{a=1}^{N-1} (\mathbf{r}_{i,a+1} - \mathbf{r}_{i,a})^2,$$

where b is the bond length and N is the number of monomers in the chain. The particle-based Hamiltonian for the system, accounting for the chain connectivity of the n amphiphiles and the pairwise energetic interactions among species, is

$$\mathcal{H} = \sum_{i=1}^n h_i(\{\mathbf{r}\}) + \frac{1}{2} \sum_{J \neq K} \int d\mathbf{r} d\mathbf{r}' \hat{\phi}_J(\mathbf{r}) u_{JK}(\mathbf{r}, \mathbf{r}') \hat{\phi}_K(\mathbf{r}').$$

In this expression, the summation is over the instantaneous density (expressed as volume fraction) of solvent (S), solvophilic (A) and solvophobic (B) monomers, defined respectively, as

$$\begin{aligned} \hat{\phi}_S(\mathbf{r}) &= v_S \sum_{j=1}^{n_S} \delta(\mathbf{r} - \mathbf{r}_j), \\ \hat{\phi}_A(\mathbf{r}) &= v_A \sum_{i=1}^{n_L} \sum_{a=1}^{N_A} \delta(\mathbf{r} - \mathbf{r}_{ia}), \\ \hat{\phi}_B(\mathbf{r}) &= 2v_B \sum_{i=1}^{n_L} \sum_{b=1}^{N_B} \delta(\mathbf{r} - \mathbf{r}_{ib}). \end{aligned}$$

We assume the pairwise interaction potential $u_{JK}(\mathbf{r}, \mathbf{r}')$ to be short-ranged, so that one may perform a gradient expansion to quadratic order as

$$\begin{aligned} u_{JK}(\mathbf{r}, \mathbf{r}') &= \\ u_{JK}(\mathbf{r}, \mathbf{r}) + \nabla u \cdot (\mathbf{r}' - \mathbf{r}) + \frac{1}{2} \nabla \nabla u : (\mathbf{r}' - \mathbf{r})(\mathbf{r}' - \mathbf{r}). \end{aligned}$$

The linear-order terms vanish by symmetry upon spatial integration. The zeroth-order terms gives to rise to the local terms and the second-order terms correspond to the square-gradient terms in eq. 2, where for simplicity, we

ignore the cross terms.

The grand canonical partition function Ξ is obtained by summing over all particle degrees of freedom, including the position of each solvent monomer, as well as the position and conformation of each lipid chain:

$$\begin{aligned} \Xi &= \sum_{n_L, n_S=0}^{\infty} \frac{e^{(\mu_L n_L + \mu_S n_S)}}{n_L! n_S! v_L^{n_L} v_S^{n_S}} \int \prod_{i=0}^{n_L} d\mathbf{r}_i \int \prod_{j=0}^{n_S} d\mathbf{r}_j \\ &\times \prod_{\mathbf{r}} \delta \left[1 - \hat{\phi}_A(\mathbf{r}) - \hat{\phi}_B(\mathbf{r}) - \hat{\phi}_S(\mathbf{r}) \right] e^{-\mathcal{H}}. \end{aligned}$$

The delta functional in the above expression accounts for the incompressibility at all positions within the system volume. The monomer volumes are used in place of the usual cube of the thermal de Broglie wavelength. This merely shifts the definition of the reference chemical potentials. In SCF theory, the first step is to replace the above particle-based model with a field-theoretic model, using a series of techniques related to Hubbard-Stratonovich transformations [?]. The microscopic density operators are converted into scalar density fields by inserting the identity

$$\int D\phi_I \delta[\phi_I(\mathbf{r}) - \hat{\phi}_I(\mathbf{r})] F[\hat{\phi}_I(\mathbf{r})] = F[\phi_I(\mathbf{r})],$$

and the delta function is in turn expressed using the Fourier representation

$$\begin{aligned} \delta[\phi_I(\mathbf{r}) - \hat{\phi}_I(\mathbf{r})] &= \\ \int D\xi_I \exp \left\{ i \int d\mathbf{r} \xi_I(\mathbf{r}) [\phi_I(\mathbf{r}) - \hat{\phi}_I(\mathbf{r})] \right\}. \end{aligned}$$

These operations decouple the interactions among particles and replace them with interactions between single molecules and effective fluctuating fields ξ_I . The grand canonical partition function can now be written as a functional integral over fluctuating fields:

$$\Xi = \int \mathcal{D}\phi_I \mathcal{D}\xi_I \exp \{-F[\phi_I, \xi_I]\}.$$

Evaluation of the functional integral by the saddle-point method leads to the self-consistent field equations with the free energy F given by eq. 2.